

Species Tag:	61004	Name:	NH ₂ CH ₂ CH ₂ OH
Version:	3		2-aminoethanol
Date:	Sept. 2003		Aminoethanol
Contributor:	B. J. Drouin		gs & 5 vibs.

Lines Listed:	282599	Q(300.0)=	141541.8102
Freq. (GHz) <	999	Q(225.0)=	75268.0205
Max. J:	60	Q(150.0)=	30180.0849
LOGSTR0=	-12.0	Q(75.00)=	6904.8309
LOGSTR1=	-10.0	Q(37.50)=	2065.3375
Isotope Corr.:	0.	Q(18.75)=	716.8160
Egy. (cm ⁻¹) >	0.0	Q(9.375)=	254.2935
μ_a =	2.65	A=	14508.72725
μ_b =	0.89	B=	5546.49379
μ_c =	0.42	C=	4570.48697

The experimental frequencies are from: R. E. Penn, R. F. J. Curl, 1971, Chem. Phys. **53**, 651 - 658; V. K. Kaushik, R.C. Woods, 1982, Z. Phys. Chem. Neue Fol **132**, 117; S. L. Widicus, B. J. Drouin, K. A. Dyl, and G. A. Blake, 2003, J. Mol. Spec. **217**, 278-281.

The dipole moment for the ground state was also reported by Penn and Curl, these values were assumed for all vibrational modes.

The v quantum numbers assign the following: 0 is the ground state, 1 is ν_{27} , 2 is ν_{26} , 3 is ν_{25} , 4 is the overtone $2\nu_{27}$, 5 is the combination $\nu_{26} + \nu_{27}$, and 6 is the combination $\nu_{25} + \nu_{27}$. The labels and energies follow the work of M. V. Korolevich et. al, 1987, Z. Prikl. Spektrosk. **46**, 620. Partition sums are explicitly calculated for the listed energy levels only and represent a partial rotation-vibration partition function that was calculated with rotational states included to J = 200 for accuracy.